6-((E)-2-Methylbut-2-enamido)hexyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C16H27NO3/c1-5-13(3)15(18)17-11-9-7-8-10-12-20-16(19)14(4)6-2/h5-6H,7-1

InchiKey: GHZZKGYIXASYDS-ACFHMISVSA-N

Formula: C16H27NO3

SMILES: CC=C(C)C(=O)NCCCCCCOC(=O)C(C)=CC

Mol. weight [g/mol]: 281.39

Physical Properties

Property code	Value	Unit	Source
gf	-46.27	kJ/mol	Joback Method
hf	-462.62	kJ/mol	Joback Method
hfus	44.46	kJ/mol	Joback Method
hvap	73.62	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.139		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	753.89	K	Joback Method
tc	946.07	K	Joback Method
tf	406.75	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.93	J/mol×K	753.89	Joback Method
cpg	731.58	J/mol×K	785.92	Joback Method
cpg	746.37	J/mol×K	817.95	Joback Method
cpg	760.37	J/mol×K	849.98	Joback Method
cpg	773.61	J/mol×K	882.01	Joback Method
cpg	786.12	J/mol×K	914.04	Joback Method
cpg	797.97	J/mol×K	946.07	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373736&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume